

SAM Co-Development to Support Fluoride-saltcooled High-temperature Reactor Design and Licensing

Final CRADA Report

Nuclear Science and Engineering Division

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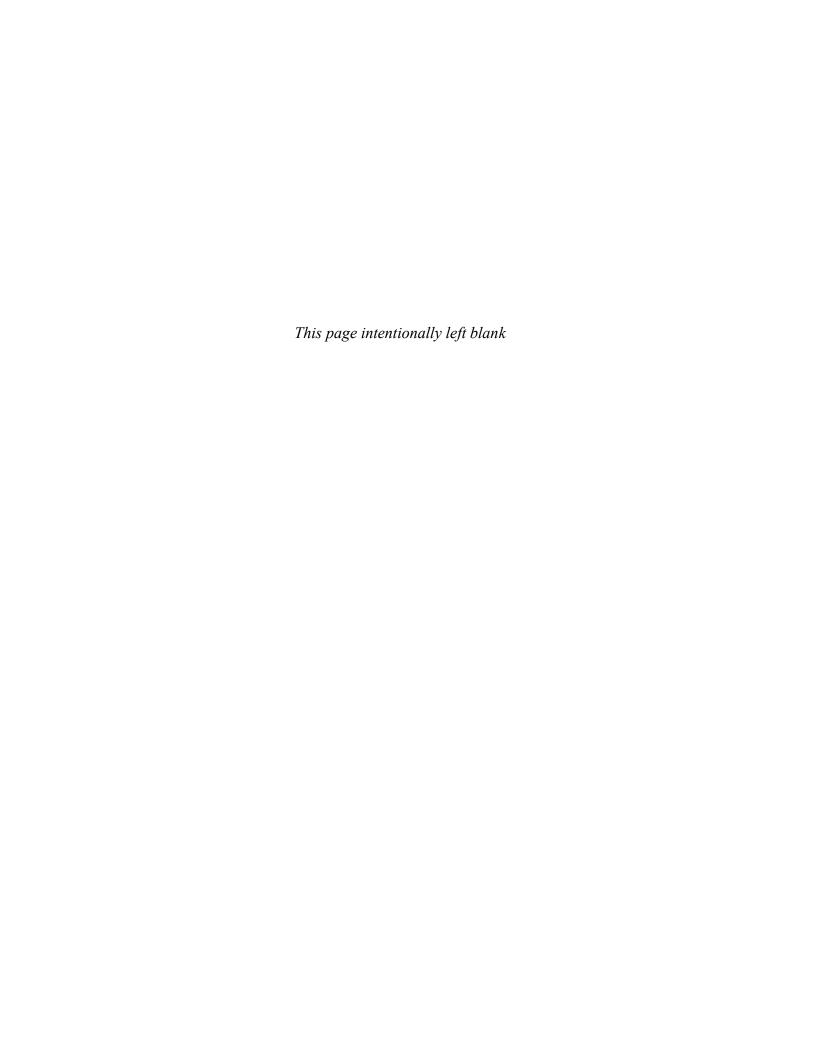
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Participants: Kairos Power, LLC

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Non Proprietary Final CRADA Report

For the Office of Scientific and Technical Information (OSTI)

CRADA Number: 2018-18177

CRADA Title: SAM Co-Development to Support Fluoride-salt-cooled High-temperature Reactor Design

and Licensing

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DOE Program or Other Government Support Program office: DOE Office of Technology Transfer

Program manager name:

Program manager phone or email:

Participant(s)

Participant 1 name: Kairos Power, LLC

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Participant 3 name: Complete address:

Argonne National Laboratory

Argonne PI(s): Rui Hu

Funding Table

To add rows, right-click in bottom row and select "Insert" "rows above".

	Planned Funding	Actual Funding	In-Kind
Government	750,000\$	750,000\$	
Kairos Power, LLC	750,000\$	\$	750,000\$
	\$	\$	\$
	\$	\$	\$
Total	1,500,000\$	750,000\$	750,000\$

Nature of Work

Describe the research (summary of Scope of Work and principal objectives of the CRADA):

This project aims to raise the SAM code's technical and commercial maturity level to enable the Kairos Power ("Kairos") to use SAM to support its KP-FHR design analysis and licensing application. Argonne National Laboratory ("Argonne") has actively developed and maintained SAM, a modern system-level analysis tool for advanced non-light water reactors safety analysis. Kairos is currently actively pursuing development of an FHR design and associated technology, and consequently requires a pedigreed safety analysis tool. The purpose of this project is to increase the maturity of the SAM code for the modeling and simulation of the KP-FHR design, thus enabling its use in safety analyses that support licensing application. Argonne will primarily be responsible for software design, development, and testing; while Kairos will be responsible for software requirements, assessment of software capabilities, needs, gaps, and priorities, and development of proprietary models. The research and development activities for the joint SAM development project include: a series of identification and prioritization studies on design

characteristics, event sequences, relevant phenomena, and software capabilities; SAM capability enhancements for specific KP-FHR systems and components; performing code verification and validations; integrating uncertainty quantification (UQ), model calibration, and sensitivity analysis (SA) techniques in safety analyses; and raising the software quality rigor level for commercial-grade applications.

DOE mission area(s):

Energy and Environmental Science and Technology Choose an item.

Choose an item.

Conclusions drawn from this CRADA; include any major accomplishments:

1. PIRT Development

A series of Kairos Power Phenomena Identification and Ranking Table (PIRT) processes were executed in the early phases of Conceptual Design for the Kairos Power Fluoride-salt-cooled, High-temperature Reactor (KP-FHR). Among them is the thermal fluids PIRT, which will provide priority for the systems code development, safety analysis, Separate Effect Tests (SETs) and Integral Effect Tests (IETs), and validation.

The PIRT process is an integral part of the Evaluation Model Development and Assessment Process (EMDAP) laid out in U.S. NRC Regulatory Guide 1.203. A PIRT relies on expert judgment to identify and rank key phenomena for a specific system undergoing a specific time phase of a specific transient. The PIRT process generates a prioritized list of key phenomena that need to be characterized and modeled to predict response to specific transients. It also ranks the knowledge level for each key phenomenon for each component, thus identifying critical gaps in the understanding of specific phenomena.

The PIRT process has been applied to reactors in operation, or reactors for which detailed engineering design exists, and for reactor designs where a wider base of expert knowledge exists. For KP-FHR safety analysis, the PIRT process is leveraged much earlier in the design of the reactor, which allows for integration of safety analysis early on in reactor design and feedback to increase the simplicity and predictability of KP-FHR transient response across a range of reference initiating events. The method is applied to a system where detailed design does not yet exist and where a large number of design options remain and are developed in parallel. Because of uncertainties in the design, the PIRT is broader than historical precedents, but for that reason, it will remain applicable as the design details are refined.

A KP-FHR Thermal-fluids PIRT report [1] has been developed based on the inputs from both internal and external PIRT review processes. The highly ranked phenomena list is basically consistent with the PIRT results developed by university led IRP FHR research projects, except for special design features for KP-FHR. Since PIRTs rely heavily on expert opinion, the Thermal-fluids PIRT will be reassessed and updated as experimental data is collected and sensitivity studies are performed.

2. SAM capability enhancements

2.1 Code Robustness enhancements

The robustness of SAM was significantly improved by resolving the code convergence issue and the mass/energy imbalance issue. Both of these two issues were related to the use of nodal boundary conditions (BC) in various boundary and junction components. These issues were resolved by adjusting the boundary

condition modeling in the boundary and junction components. The feedback from various users confirmed that these updates improved significantly the robustness of SAM code.

It had been found and reported that the SAM code may experience convergence problems for certain test cases or input models. These test cases might run well for certain time (such as hundreds of seconds) but then failed for no obvious reasons due to convergence. The simulation results before the failed timestep seemed reasonable. A study was then performed to closely examine the code convergence using a number of test cases. It was found that the convergence issue was related to the boundary condition modeling in boundary and junction components. The use of nodal BC could cause large discontinuity in the residual function if there is a flow reversal event during the transient. This large discontinuity cannot be resolved by the Newton's method with an adaptive time step decrease mechanism and causes a convergence trap, see Figure 1. The study confirmed that this convergence trap can be avoided by switching the nodal BC to the integral BC during the transient simulations.

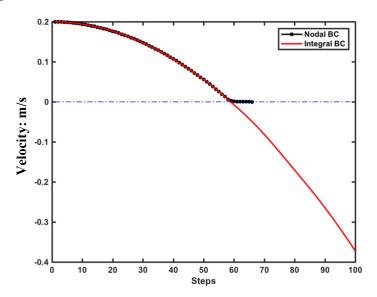


Figure 1. Convergence trap due to the combination of flow reversal event and nodal boundary condition

It had been found and reported that the SAM code may experience small mass/energy imbalance issues for certain test cases. The mass/energy imbalance issues were not acceptable in long-time power plant simulations, because the mass/energy imbalance issues bring in unphysical mass/energy leakage from the system. To resolve these issues, the SAM code was at first updated to add a series of postprocessors for logging the mass/energy imbalance during the transient simulations. Following this update, a sensitivity study was performed to examine these issues. It was found that the mass/energy imbalance issues were caused by the use of nodal boundary conditions for pressure variable and inconsistent mass flux boundary conditions in a few boundary and junction components, which break the weak form of the mass balance equation. The feedback from various users confirmed that these issues were successfully resolved, and the mass/energy imbalance were reduced to negligible level, see Figure 2.

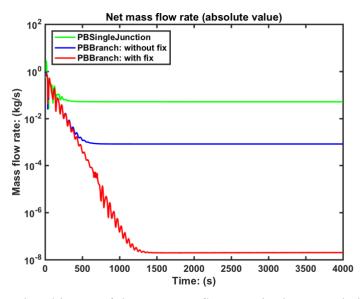


Figure 2. Transient history of the net mass flow rate in the natural circulation loop

2.2 Control and trip system modeling

Industrial control and trip system play a fundamental role in the nuclear power plant. These systems are widely used by nuclear systems and plants to automatically control various equipment and systems or provide interfaces for human operators during normal and abnormal conditions. The control system generates analogous control signals such as control rod insertion speed and valve opening or closing speed. The trip system generates digital (Boolean) signals indicating set-point actuations or events occurrences. The control and trip system models were developed and added into SAM. The development of control and trip system models has started with identifications of functional requirements and design specifications. Based on the functional requirements and design specifications, the ANL and Kairos Power teams completed tasks implementing the models, including code structure design, new input identification, and development of control and trip component models.

The hierarchy of classes of control and trip system model is shown in Figure 3, where the control and trip components are implemented as *ControlSystem* and *TripSystem* classes respectively. There are several classes further derived from *ControlSystem* such as *CSAddition*, *CSDivision*, and others, each representing a control component performing a specific operation. Similarly, there are three classes *TSBoolean*, *TSComparison*, and *TSDelay* derived from *TripSystem*, representing the trip components performing Boolean operations, comparison, and delay respectively. Users can build a control or trip system diagram flexibly by connecting the components. Testing has been performed during and after the implementation to ensure the new models are correctly implemented and code performances are reasonable, see Figure 4 for a demonstration of a mass flow rate controller.

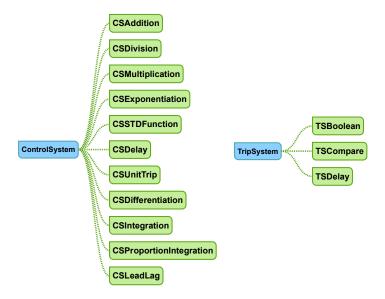


Figure 3. Hierarchy of control and trip system in SAM

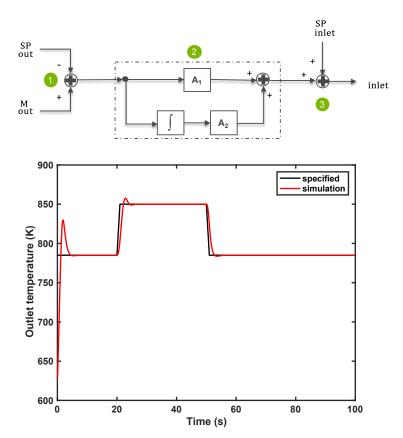


Figure 4. Mass flow rate controller (top) and demonstration result (bottom). The mass flow rate controller is designed to control the channel outlet temperature by adjusting the channel inlet mass flow rate.

2.3 Porous medium flow modeling of pebble bed

In nuclear reactor thermal-hydraulics analysis, it is a common approach to using porous medium flow to model the fluid flow and heat transfer in very complex but with regular pattern geometries, such as the pebble bed core in the HTGR and FHR designs. To support reactor core modeling and simulation needs for these types of reactor designs, a porous-medium-flow model has been implemented in SAM. The implemented model includes a set of mass, momentum, and energy balance equations for the fluid phase, and an additional energy balance equation for the solid (pebble) phase. The code implementation of these equations and necessary stabilization schemes are largely based on a previously existing multi-dimensional flow model in the SAM code, with details available in references [2] and [3].

Many porous-medium-flow closure correlations to support pebble bed core flow and heat transfer simulations have been implemented, including frictional pressure drop [4], pebble-to-fluid heat transfer and pebble-bed-to-wall heat transfer [5], and effective thermal conductivity [3] of pebble beds. Code validation efforts have also been made to validate the implemented correlations, including frictional pressure drop correlations validation using different types of fluid in a wide range of Reynolds numbers [4], effective thermal conductivity correlations validation using the experimental data from the High Temperature Test Unit (HTTU) facility [4].

In order to demonstrate and evaluate the ability of SAM porous-medium-flow model for PB-FHR designs, a two-dimensional (2D) RZ axial-symmetric model has been developed to simulate a reference FHR core that is similar to the Kairos Power design. The coupling between the 2D core model and the primary system 1D model was also achieved using MOOSE's multiApp framework, from which a steady-state solution was obtained, as shown in the figure below. Continuous improvements are being made to enhance the fidelity of pebble temperature distribution and the coupling between SAM multi-D fluid flow and 1D models.

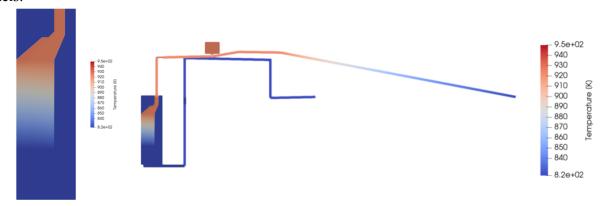


Figure 5. Steady state solution of fluid temperature in a reference FHR model, left: 2D RZ axial-symmetric model; right: coupled 2D/1D temperature profile at steady state.

2.4 Overview of capability enhancements at KP

In order to simulate KP-FHR specific features, additional models and components [6] have been developed beyond the models provided by SAM. The enhancements include special component models such as pebble bed core channel component (*PebbleBedCoreChannel*), Tank component, and Twisted Elliptical Tube Heat Exchanger component (*TwistedTubeHX*); proprietary closure models for heat transfer and wall friction models; and solid and fluid properties.

PebbleBedCoreChannel is a component that models 1-D flow and heat transfer through a pebble bed reactor core. This component allows a core channel to be modeled with 1-D spherical fuel elements. ANL-1060 (07/17/2019)

TRISO particle fuel temperature model is added in KP-SAM to evaluate temperatures in the particles, in addition to the average solid temperature at the fuel annulus evaluated by KP-SAM 1-D spherical heat structure model. In this way, multiple scale temperature information can be obtained.

The tank model as shown in Figure 6 simulates a finite, time-dependent zero-dimensional volume where the level of salt in the volume can increase and decrease as salt flows into or out of the volume. The model supports an arbitrary number of one-dimensional flow connections, i.e. pipes, to the zero dimensional volume, but currently does not support the handling of situations where pipe inlets become covered or uncovered during transient simulation. The model includes the capability to simulate an ideal compressible gas in the upper space of the tank where salt is not present. The tank model can simulate inertial effects associated with the thermal mass of the tank walls. Convective heat transfer coefficients for energy transfer between the constituent sub-areas of the tank model may either be specified as constants or calculated through the specification of appropriate correlations.

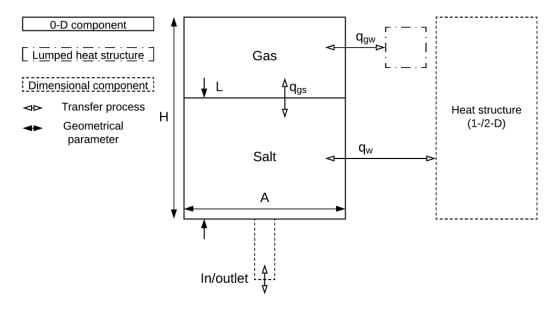


Figure 6. Schematic of Tank component in KP-SAM

TwistedTubeHX is a component that models flow and heat transfer through a twisted elliptical tube heat exchanger, one of the major candidate designs for the intermediate heat exchanger. This component allows higher fidelity modelling than can be achieved via PBHeatExchanger and removes most potential for user error in describing the complicated geometry of twisted elliptical tubes. TwistedTubeHX is an assembly component consisting of two PBHeatExchanger components, one PBCoupledHeatStructure component, and four PBVolumeBranch components. Special heat transfer correlations for twisted elliptical tube geometry have been implemented based on Kairos Power SET test.

3. SAM Assessment

A detailed KP-SAM verification and validation (V&V) report [7] has been developed which provides a long term, comprehensive plan to verify and validate KP-SAM so that it can be used for licensing safety analysis. As part of KP-SAM development, V&V also follow U.S. NRC's Evaluation Model Development and Assessment Process (EMDAP). The iterative and layered V&V methods begin with simple software verification to cover each newly developed physical component or additional new functions for the component. Strict numerical verification checks the order of convergence for field equations for both time ANL-1060 (07/17/2019)

and space. Unit test covers simple test data and is used to validate fluid and solid properties, and heat transfer and wall friction correlations. SET validation covers all the important AOO and DBE relevant TH phenomena identified by the PIRT report, plus additional fundamental models validation. IET validation covers scaled integral tests at system level or plant level. Reactor tests provide more direct evidence that the systems code can accurately simulate transient responses. Uncertainty Quantification process will follow EMDAP to quantify all the important uncertainties. Because the KP-FHR design is still in the conceptual stage and detailed design feature and information can only be available in the next design stage, this plan only covers the preliminary thermal hydraulic phenomena and design features with reasonable expectation to be important according to current thermal fluid PIRT report. This plan provides general guidance for KP-SAM software and numerical verification efforts and provides a base to develop SETs, IETs, and tests performed at Hermes test reactor. This plan will be routinely updated according to the design progress.

Kairos Power has finished majority of verification work for KP-SAM required by the KP-SAM V&V plan. The only validation work completed by KP-SAM team is the preliminary validation for twisted elliptical tube heat exchanger test (Eurydice II Test) [8]. The purpose of this study is the formulation and validation of shell-side Nusselt number and friction factor correlations in the twisted elliptical tube (TET) heat exchanger model. This model makes use of special geometric considerations and unique-to-Kairos closure relations to simulate six experiments run by the KP testing team (Eurydice II experiments). These closure relations are developed based on the experimental data and are found to apply well across a range of Reynolds and Prandtl numbers. While the contents of these experiments do not provide a complete set of metrics to validate the model over a wide enough range of conditions, the current state is useful for testing validation practices in KP-SAM and demonstrating the code's ability to closely match realistic transient behavior.

In order to establish confidence in predictions and to quantify the uncertainty in SAM calculations, a significant V&V effort is also pursued at Argonne. Rigorous validation activities have been performed against a number of experiment facilities or test reactors. A validation report [9] was created to summarizes a few validation activities utilizing experimental test cases in the following test facilities:

- 1. Compact Integral Effects Test (CIET) facility at UC Berkeley,
- 2. University of Minnesota Water-Based Natural Circulation Loop,
- 3. Experimental Breeder Reactor-II (EBR-II),
- 4. Natural Convection Shutdown Heat Removal Test Facility (NSTF),
- 5. Low-temperature DRACS test facility (LTDF) at the Ohio State University.

Four of the five validation cases show excellent agreement between the SAM predictions and the experimental results. The fifth case, the LTDF study, requires additional work to improve the simulation convergence and refine the comparisons at the early stages of each transient.

In order to allow for automated reproducibility, the validation report was created using GNU Make, PYTHON and LaTeX. For each of the above validation cases, SAM input files were created. Each SAM input file has a corresponding python post processing script and a CSV file containing the experimental results to be used for comparisons. The post processing scripts were designed to combine the SAM predictions and experimental results into figures according to plotting functions. Together with the created figures, a LaTeX file for each validation case will be compiled and the complete validation report will be created. A GNU Makefile for each validation case monitors changes in the SAM executable, SAM input/output files, and LaTeX files, executing the appropriate subsequent steps each time a dependency is updated. This framework allows for the validation report to be periodically updated with relatively little

effort. In the event that the SAM predictions change, a comparison of the previous and updated predictions will be created, a warning message will be printed to the screen, and post processing will exit before updating the figures. After the code manager has reviewed the comparison, the updated solutions can be approved, and post processing can continue.

4. SAM-Dakota Integration

Advancements in the knowledge of nuclear reactor performance have led to an increased need to perform Sensitivity Analysis (SA) and Uncertainty Quantification (UQ) in the advanced reactor domain. The role of uncertainty quantification spans many facets in the nuclear industry, including system design and optimization, licensing, and probabilistic risk assessment. The Dakota software, maintained by Sandia National Laboratory, is an uncertainty quantification and optimization toolkit that has been in development for over 20 years [10]. Work was performed to integrate SAM and Dakota, achieved through a Python coupling framework, in order to leverage the sensitivity analysis, uncertainty quantification, and other statistical tools that make up Dakota.

At the base level, Dakota interfaces with the code in a black-box fashion, using system calls to initiate simulations with SAM. Data communication between Dakota and the external code occurs through parameter and response files. The framework parses a SAM template input file and replaces the uncertain parameters with the random values generated by Dakota. Once all SAM inputs are generated, execution can be handled either on a single node using Dakota's built-in management schemes, or they can be handled on multiple nodes by batching and submission to a cluster queue to be handled by a scheduler on an HPC.

After the SAM simulations complete, the Python interface parses the output CSV file for the target responses. The built-in filters can process the SAM simulation results to process the maximum, minimum, starting, or final value of an output parameter to be provided back to Dakota. Users can choose the parameters or response variables on which these filters are applied. These responses of interest are written in a result file and sent back to Dakota for statistical analysis.

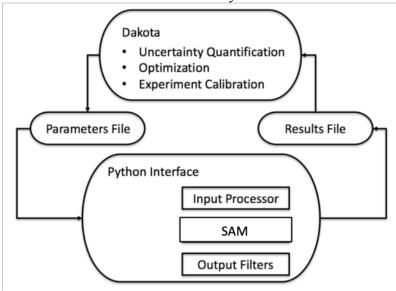


Figure 7.SAM-Dakota coupling scheme.

The coupling framework is provided through two examples that are included in the SAM code package with additional documentation included in the User's Guide. This framework has been used to perform uncertainty quantification studies of the EBR-II benchmark problem [11].

5. Software Quality Assurance

The SAM software quality assurance (SQA) program framework has been developed with the goal of meeting the needs of end-users completing DOE authorization or NRC licensing of an advanced reactor design. Because it is expected that this effort will occur over an extended period as resources permit, a phased approach to SQA Program development is being executed to leverage the resources available at each phase and to reduce any obstacles to efficient SQA Program sustainment. The initial phase of SQA Program development is focused on satisfying fundamental SQA best practices. A hierarchical document structure has been adopted for the SAM SQA Program, with a central SQA Plan (SQAP) comprising the top level of the Program. The SAM SQAP adopts the MOOSE SQAP. It delineates the SQA Program framework for SAM by describing the Program activities, organization, and documentation, and by clearly defining the interconnection of all Program items. Compliance to the SQAP is required throughout the software life cycle, including planning, requirements, acquisition, design, implementation, acceptance testing, maintenance and operations, and retirement.

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- 2. L. Zou, D. Nunez, and R. Hu, Development and Validation of SAM Multi-dimensional Flow Model for Thermal Mixing and Stratification Modeling, ANL/NSE-20/19, June 2020, Argonne National Laboratory.
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- 11. T. Mui and R. Hu, "Uncertainty Quantification Study on EBR-II Benchmark Modeling Strategies using SAM," ANS Virtual Winter Meeting 2020, November 16-19, 2020.

Technology Transfer-Intellectual Property Argonne National Laboratory background IP:

SAM reactor system analysis code

Participant(s) background IP:

KP-SAM reactor system analysis code

Identify any new Subject Inventions as a result of this CRADA:

N/A

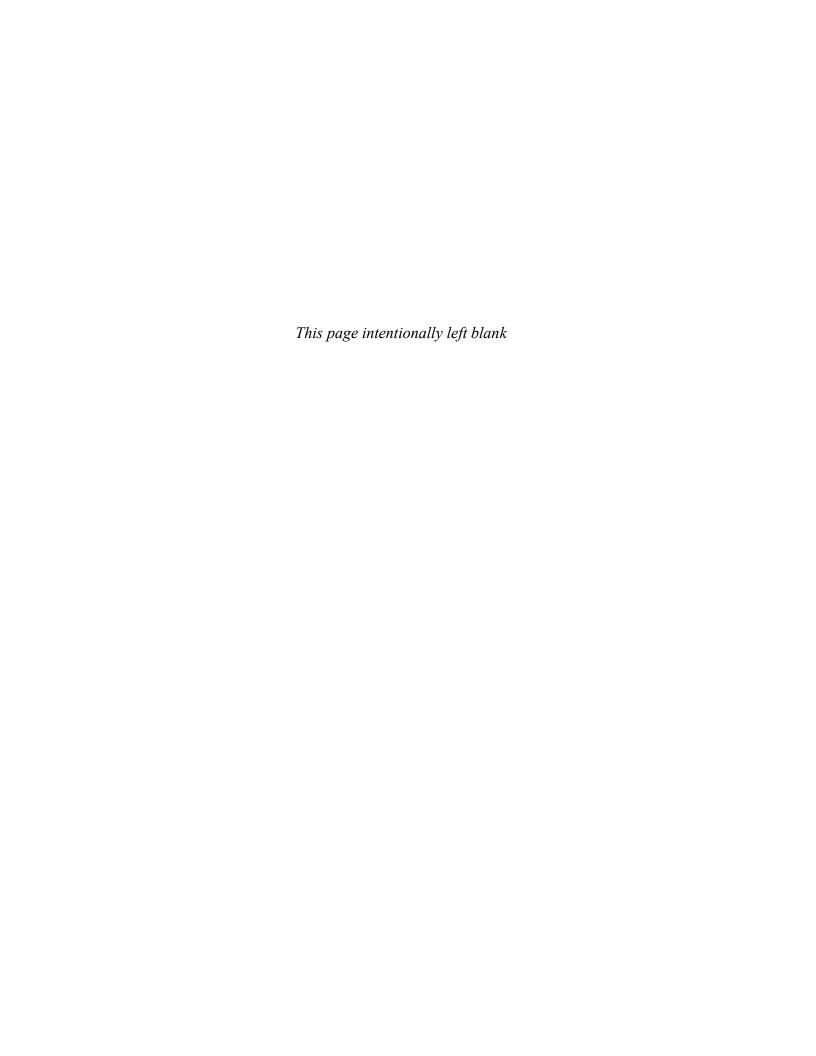
Summary of technology transfer benefits to industry and, if applicable, path forward/anticipated next steps towards commercialization:

The work performed was instrumental in improving SAM code capabilities and maturities for its use for design and licensing simulation of Flouride Salt Cooled High Temperature Reactors (FHRs). Kairos has adopted SAM, and is developing its proprietary version (KP-SAM) for the licensing application of its reactor technology. This has significant benefit in terms of increased use of the SAM code as well as accelerated development of a promising reactor technology.

Other information/results (papers, inventions, software, etc.):

Papers/Reports

- 1. E. Blandford, K. Brumback, L. Fick, C. Gerardi, B. Haugh, E. Hillstrom, K. Johnson, P.F. Peterson, F. Rubio, F. Sarikurt, S. Sen, H. Zhao, N. Zweibaum, Kairos Power Thermal Hydraulics Research and Development, *Nuclear Engineering and Design*, Vol. 364, 2020. https://doi.org/10.1016/j.nucengdes.2020.110636.
- 2. H. Zhao, L. Fick, J. Herter and B. Haugh, "Overview of Kairos Power Systems Code KP-SAM Development,", *Proceedings of 18th International Topical Meeting on Nuclear Reactor Thermal Hydraulics*, Portland, OR, 2019.
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- 5. Zou, Ling and Rui Hu. "Validation of SAM using CIET Experimental Data." 2019 American Nuclear Society Winter Meeting, Washington, DC US, November 17- 21, 2019.
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